electron configuration

Electron Configuration

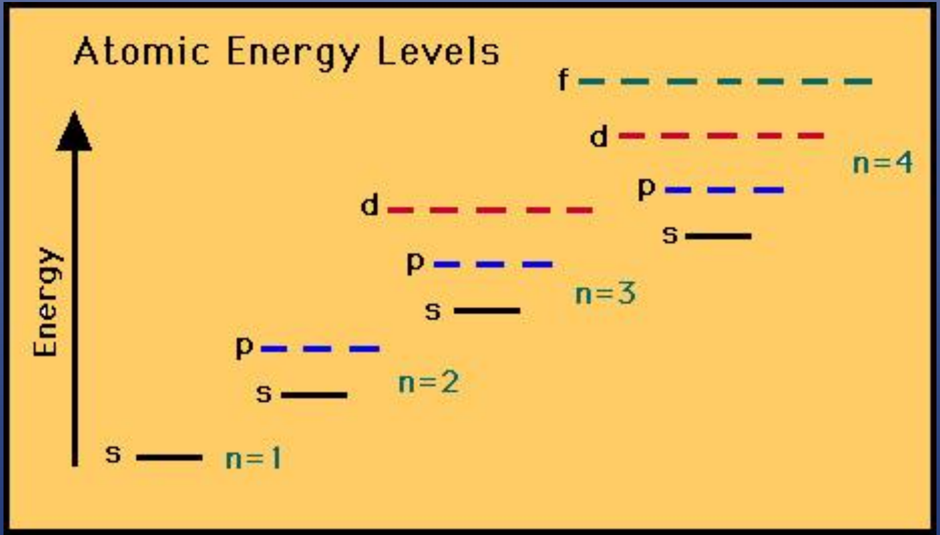
- Knowing the arrangement of electrons in atoms will better help you understand chemical reactivity and predict an atom's reaction behavior.
- We know when n=1 (1st EL), there are 2 e^- ($2n^2$); n=2, 8 e^-, n=3, 18 e^-, etc. …
BUT what SUBLEVEL and ORBITAL are these electrons in?

Electron Configuration: way electrons are arranged in various orbitals around the nuclei of atoms

Electron Configuration

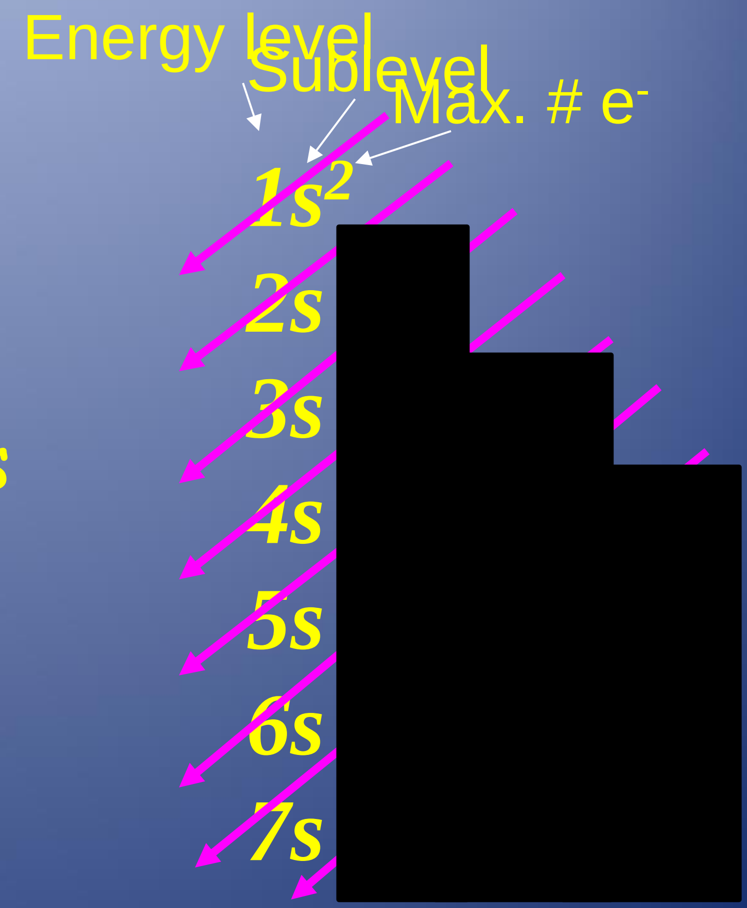
Rules that govern electron configuration

1. Aufbau Principle: electrons enter the lowest energy state possible
2. Pauli Exclusion Principle: at most 2 electrons per orbital; these must have opposite spins
3. Hund's Rule: electrons do not pair until each orbital in a sublevel has at least 1 electron



Electron Configuration Notation

NOTATION: The notation for a configuration lists the energy level, followed by the sublevel symbols, one after the other, with a superscript giving the number of electrons in that sublevel.



[redacted]

e.g. Nitrogen

\# electrons

[redacted]

Energy Level

Sublevel

Distributing Electrons in the Atom

- Write the electron configurations for silicon, scandium, and chromium

Silicon (14 e^-)

$1s^2 2s^2 2p^6 3s^2 3p^2$

Scandium (21 e^-)

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^1$

Chromium (24 e^-)

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^4$

Expected-But this is not what happens!!!

Exceptional Electron Configurations

- Atoms with full outer EL's are particularly stable (less reactive)
- In addition to full outer EL's, there are other e^- configurations of high relative stability: *filled sublevels*
- Some actual electron configurations differ from those assigned using the Aufbau Principle because half-filled sublevels are not as stable as filled sublevels, but they are more stable than other configurations.
- Exceptions to the Aufbau Principle are due to subtle electron-electron interactions in orbitals with very similar energies.

Exceptional Electron Configurations

Chromium is actually:

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^5$

Why?

- This gives us two half filled orbitals (the others are all still full)
- Half full is slightly lower in energy.
- The same principal applies to copper.

Exceptional Electron Configurations

Copper has 29 electrons so we expect:

$$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^9$$

- But the *actual configuration* is:

$$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^{10}$$

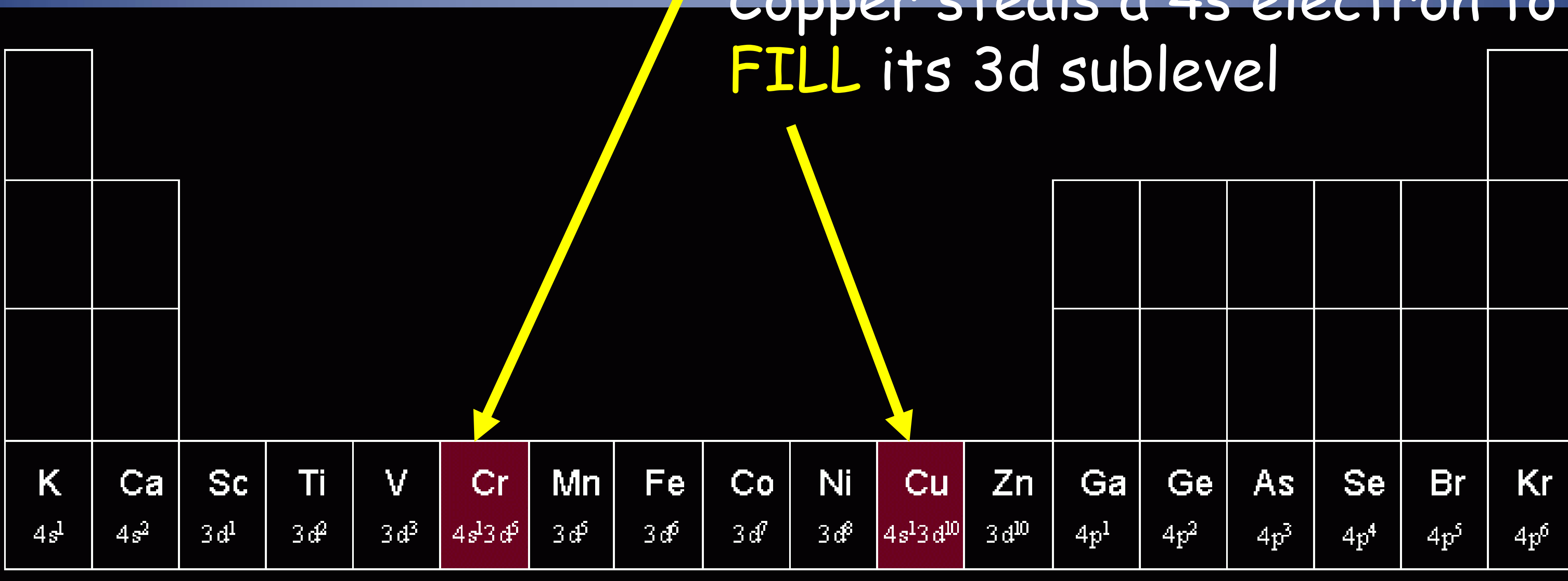
- This change gives one more filled orbital and one that is half filled.

Remember these exceptions: d^4, d^9

Exceptional Electron Configurations

Chromium steals a 4s electron to make its 3d sublevel HALF FULL

Copper steals a 4s electron to FILL its 3d sublevel



Noble Gas Configuration

A few terms to define to understand this more fully…

- *Valence shell*: outermost EL that is occupied by e^- in the electron cloud
- *Valence shell electrons*: an e^- that is available to be lost, gained, or shared in the outer EL
  - These electrons are of primary concern because they are the electrons most involved in chemical reactions.

$1s^2$ $\underline{2s^2}$ $\underline{2p^3}$

Valence shell = 2nd EL

Valence shell e^- = 5

Noble Gas Configuration

Noble Gas Configuration: abbreviated form of e^- configuration which avoids writing "inner e^-" and therefore only requires writing valence shell e^-

- NOTATION: The notation for noble gas configuration lists the elemental symbol of the nearest noble gas (Group VIII A (18) elements- *helium, neon, argon, krypton, xenon, and radon*) in brackets, followed by the electron configuration of the *valence electrons*

  e.g. Nitrogen

  nearest noble gas is Helium

  [He] $2s^2$ $2p^3$

  [He] represents the "inner electrons" ($1s^2$)

PRACTICE: Noble Gas Configuration

- Write the noble gas configurations for silicon, scandium, and chromium.

Silicon

Scandium

Chromium

Electron Dot Diagram (Lewis Dot)

Electron Dot Diagram: the representation of an atom in which an element stands for the nucleus and dots are used to represent the valence shell electrons of this atom

Electron Dot Diagram (Lewis Dot)

e.g. Nitrogen

$1s^2\ 2s^2\ 2p^3$

5 valence e^-

To draw electron dot diagrams:

1. Determine the **electron configuration** of the element.
2. Determine the number of **valence electrons**.
3. Write the **atomic symbol** of the element.
4. Place **1 dot per e^-** on each side moving clockwise.
5. When each side has 1 e^-, place a second dot on each side, again moving clockwise.

There can be a **maximum of 8 dots** around an element.

PRACTICE: Electron Dot Diagrams

- Draw the electron dot diagrams for silicon, scandium, and chromium.

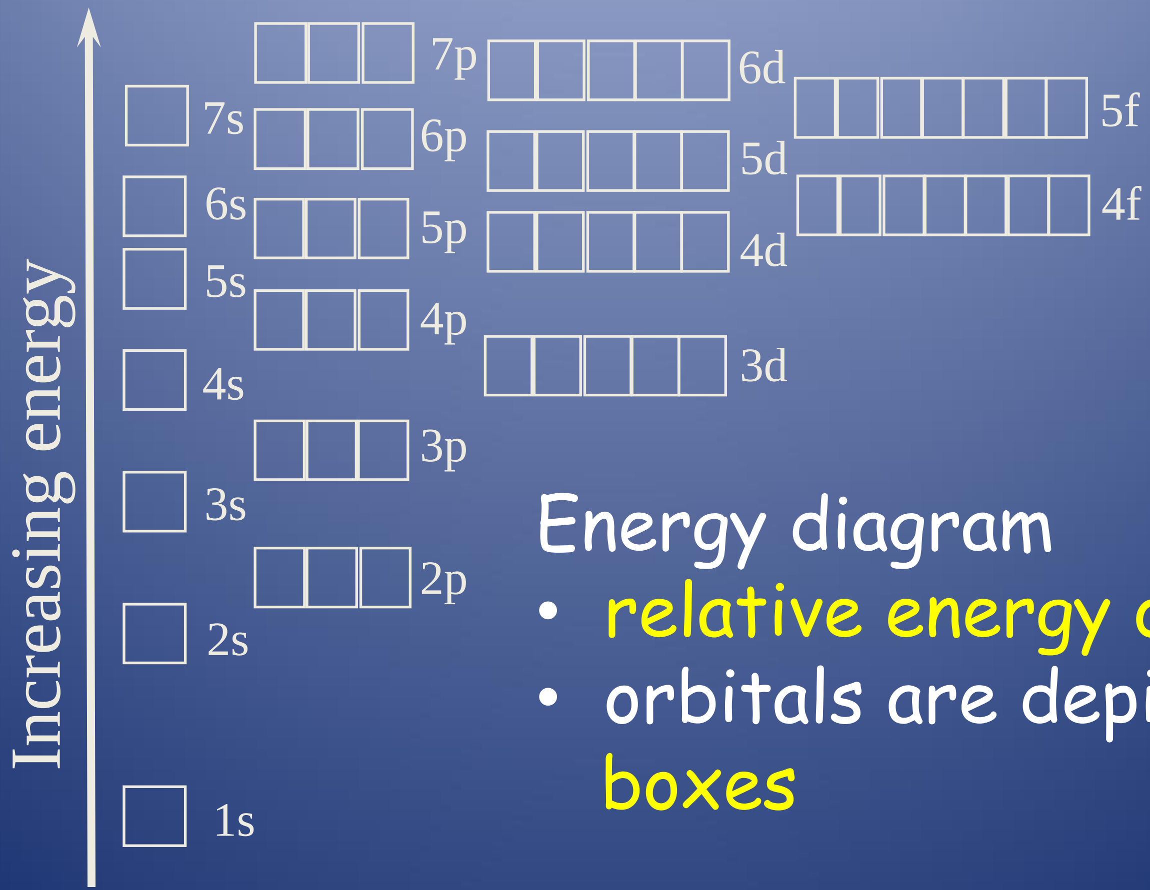
Silicon

Scandium

Chromium

Filling Patterns of Orbitals

- Finally, in discussing the arrangement of electrons in atoms, we have not yet described how the electrons are arranged within each sublevel.



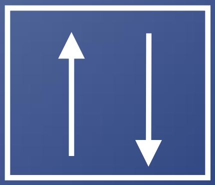
Energy diagram

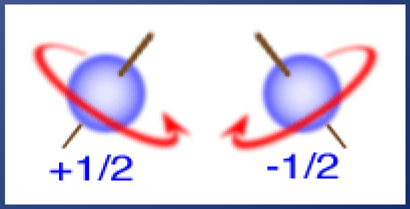
- relative energy of sublevels
- orbitals are depicted as boxes

Pauli Exclusion Principle

1924-Wolfgang Pauli

- States that atomic orbitals can have at most two electrons
- Electrons paired within an orbital must have opposite spins (+1/2, -1/2)
- Atomic orbital depicted as a box (or simply as a line or circle)
- Electrons are depicted as arrows
    - An up arrow denotes an "up" spin
    - Down arrow denotes a "down" spin

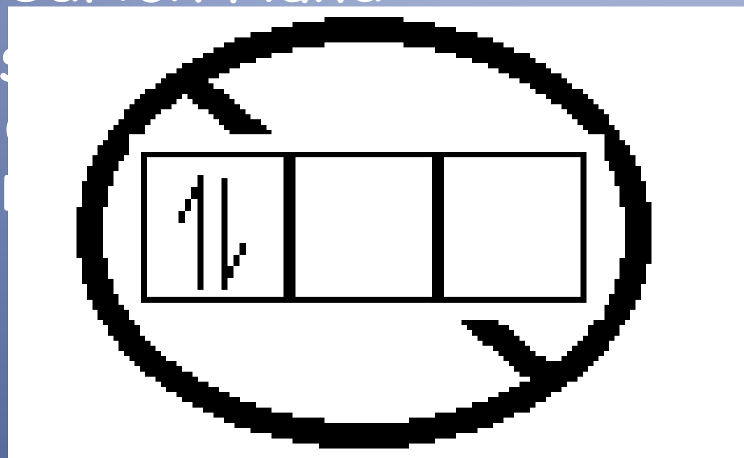


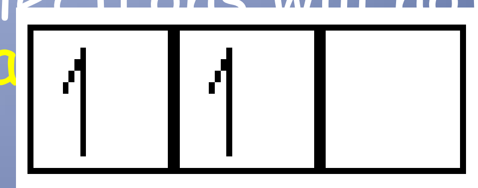


Hund's Rule

1927-Friedrich Hund

Electrons ... itals within sublevels because ... electrons will not pair until the... y a





Example: carbon's outer two electrons are in the 2p sublevel where there are three available atomic orbitals: p_x, p_y, p_z

- If the first electron enters p_x, the second electron will not pair with it in the same orbital; it will enter one of the available empty orbitals (p_y or p_z)

Filling Patterns of Atomic Orbitals

- Atomic Orbitals are filled from lowest energy to highest energy

- Full/half full atomic orbitals
  - Adding electrons until all orbitals are full is a lower energy state (usually)
  - Paired electrons are higher energy than unpaired (Hund's Rule)
  - Half full orbitals reduce electrostatic repulsion (Coulomb's Law)

Orbital Notation Diagrams

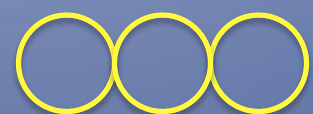
- To describe how orbital of a sublevel are occupied by electrons, we use an orbital notation diagrams.

To draw an orbital notation diagram:

1. Represent each orbital by a circle (or square or line).

s-sublevel

1s



p-sublevel

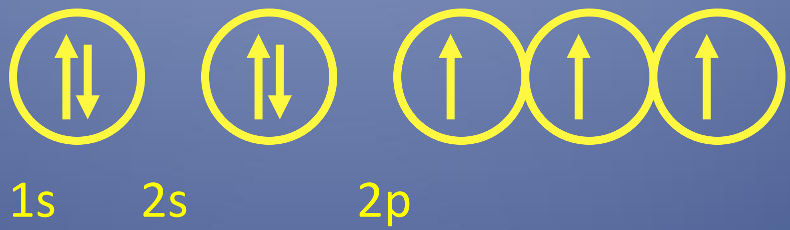
3p

1. Label each group of orbital in a sublevel with the energy level and sublevel.
2. Represent electrons within each orbital by drawing in an arrow for EACH electron (following Aufbau, Pauli, and Hund's rules)

Orbital Diagram Notation

- Therefore, applying Pauli Exclusion Principle, the Aufbau Principle, and Hund's Rule, we can see that nitrogen's orbital notation diagram is accurately represented as:

    e.g., nitrogen



PRACTICE: Orbital Notation Diagrams

- Draw the orbital notation diagrams for silicon, scandium, and chromium.

Silicon

Scandium

Chromium